Quantum Phase Transition in a Far-from-Equilibrium Steady State of an *XY* Spin Chain

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Using quantization in the Fock space of operators, we compute the nonequilibrium steady state in an open Heisenberg *XY* spin 1/2 chain of a finite but large size coupled to Markovian baths at its ends. Numerical and theoretical evidence is given for a far-from-equilibrium quantum phase transition with the spontaneous emergence of long-range order in spin-spin correlation functions, characterized by a transition from saturation to linear growth with the size of the entanglement entropy in operator space.

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The nonperturbative physics of many-body open quantum systems far from equilibrium is largely an unexplored field. In one-dimensional locally interacting quantum systems, equilibrium phase transitions—quantum phase transitions (QPTs)—can occur at zero temperature only and are by now well understood [1]. QPTs are typically characterized by vanishing of the Hamiltonian's spectral gap in the thermodynamic limit at the critical point and (logarithmic) enhancement of the entanglement entropy and other measures of quantum correlations in the ground state [2]. Much less is known about the physics of QPTs out of equilibrium, studies of which have been usually limited to near-equilibrium regimes or using involved and approximate analytical techniques (e.g., [3,4]).

There exist two general theoretical approaches to a description of nonequilibrium open quantum systems: namely, the nonequilibrium Green's function method [5] and the quantum master equation [6,7]. In this Letter, we adopt the latter and present a quasiexactly solvable example of an open Heisenberg *XY* spin 1/2 chain exhibiting a novel type of phase transition far from equilibrium, characterized by a sudden appearance of long-range magnetic order in the nonequilibrium steady state (NESS) as the magnetic field is reduced, and the transition from saturation to linear growth with the size of the operator space entanglement entropy (OSEE) of NESS.

The Hamiltonian of the quantum *XY* chain reads

$$H = \sum_{m=1}^{n-1}\left(\frac{1+\gamma}{2}\sigma^x_m\sigma^x_{m+1} + \frac{1-\gamma}{2}\sigma^y_m\sigma^y_{m+1}\right) + \sum_{m=1}^{n} h\sigma^z_m, \tag{1}$$

where $\sigma^{x,y,z}_m$, $m = 1, \ldots, n$, are Pauli operators acting on a string of n spins. We may assume that parameters γ (anisotropy) and h (magnetic field) are non-negative. It is known that *XY* model (1) exhibits (equilibrium) critical behavior in the thermodynamic limit $n \to \infty$ along the lines $\gamma = 0$, $h \le 1$, and $h = 1$. Here we consider an open *XY* chain whose density matrix evolution $\rho(t)$ is governed by the Lindblad master equation [6] (we set $\hbar = 1$)

$$\frac{d\rho}{dt} = \hat{\mathcal{L}}\rho := -i[H,\rho] + \sum_{\mu=1}^{M}(2L_\mu\rho L_\mu^\dagger - \{L_\mu^\dagger L_\mu, \rho\}) \tag{2}$$

and study a phase transition in NESS. The simplest nontrivial bath (Lindblad) operators acting only on the first and the last spin are chosen ($M = 4$):

$$L_{1,2} = \sqrt{\Gamma^L_{1,2}}\sigma^{\mp}_1, \qquad L_{3,4} = \sqrt{\Gamma^R_{1,2}}\sigma^{\mp}_n, \tag{3}$$

where $\sigma^{\pm}_m = (\sigma^x_m \pm i\sigma^y_m)/2$ [8]. For $h \gg 1$, the ratios $\Gamma^\lambda_2/\Gamma^\lambda_1 = \exp(-2h/T_\lambda)$ are simply related to canonical temperatures of the end spins T_λ, $\lambda = L, R$.

Note that Lindblad equation (2) can be rigorously derived within the so-called Markov approximation [7], which is justified for macroscopic baths with fast internal relaxation times. As shown in Ref. [9], Eq. (2) with (1) and (3) can be solved exactly in terms of normal master modes (NMMs), which are obtained from diagonalization of $4n \times 4n$ matrix $\mathbf{A}$ written in terms of 4×4 blocks

$$\mathbf{A}_{l,m} = \delta_{l,m}(-2h\mathbf{R}_0 + \delta_{l,1}\mathbf{B}_L + \delta_{l,n}\mathbf{B}_R) + \delta_{l+1,m}\mathbf{R}_\gamma - \delta_{l-1,m}\mathbf{R}^T_\gamma, \quad l, m = 1, \ldots, n, \tag{4}$$

where $\mathbf{R}_\gamma = \mathbb{1}_2 \otimes (i\sigma^y - \gamma\sigma^x)/2$ and $\mathbf{B}_\lambda = -\frac{1}{2} \times (\Gamma^\lambda_2 + \Gamma^\lambda_1)\sigma^y \otimes \mathbb{1}_2 + \frac{1}{2}(\Gamma^\lambda_2 - \Gamma^\lambda_1)(\sigma^z + i\sigma^x) \otimes \sigma^y$.

Following Ref. [9], the key concept is 4^n-dimensional Fock space of operators $\mathcal{K}$ spanned by an orthonormal basis $P_{\alpha_1,\ldots,\alpha_{2n}} := w_1^{\alpha_1}\ldots w_{2n}^{\alpha_{2n}}$, $\alpha_j \in \{0, 1\}$, where $w_{2m-1} = \sigma^x_m\prod_{m'<m}\sigma^z_{m'}$ and $w_{2m} = \sigma^y_m\prod_{m'<m}\sigma^z_{m'}$ are anticommuting operators $\{w_j, w_k\} = 2\delta_{j,k}$. We introduce canonical adjoint Fermi maps over $\mathcal{K}$, defined as $\hat{c}_j|P_{\underline{\alpha}}\rangle = \delta_{\alpha_j,1}|w_jP_{\underline{\alpha}}\rangle$, so the quantum Liouvillean (2) becomes bilinear $\hat{\mathcal{L}} = \underline{\hat{a}} \cdot \mathbf{A}\underline{\hat{a}} + \mathrm{const}\mathbb{1}$ in Hermitian maps $\hat{a}_{2j-1} = (1/\sqrt{2})(\hat{c}_j + \hat{c}_j^\dagger)$ and $\hat{a}_{2j} = (i/\sqrt{2})(\hat{c}_j - \hat{c}_j^\dagger)$, satisfying $\{\hat{a}_p, \hat{a}_q\} = \delta_{p,q}$. The eigenvalues of $4n \times 4n$ antisymmetric matrix $\mathbf{A}$ (4) called rapidities come in pairs $\beta_1, -\beta_1, \ldots, \beta_{2n}, -\beta_{2n}$, $\mathrm{Re}\beta_j \ge 0$. The corresponding eigenvectors $\underline{v}_p$, $p = 1, \ldots, 4n$, defined by $\mathbf{A}\underline{v}_{2j-1} = \beta_j\underline{v}_{2j-1}$ and $\mathbf{A}\underline{v}_{2j} = -\beta_j\underline{v}_{2j}$, can always be normalized as $\underline{v}_{2j-1}\cdot\underline{v}_{2j} = 1$ and $\underline{v}_p\cdot\underline{v}_q = 0$ otherwise. Writing NMM maps as $\hat{b}_j = \underline{v}_{2j-1}\cdot\underline{\hat{a}}$ and $\hat{b}'_j = \underline{v}_{2j}\cdot\underline{\hat{a}}$, in general $\hat{b}'_j \ne \hat{b}^\dagger_j$, obeying $\{\hat{b}_j, \hat{b}_k\} = \{\hat{b}'_j, \hat{b}'_k\} = 0$ and $\{\hat{b}_j, \hat{b}'_k\} = \delta_{jk}$, the Liouvillean (2) takes the normal form $\hat{\mathcal{L}} = -2\sum_{j=1}^{2n}\beta_j\hat{b}'_j\hat{b}_j$. Thus a complete set of 4^n eigenvalues

of $\hat{\mathcal{L}}$ (real parts being the relaxation rates) can be constructed as $-2\sum_j \nu_j \beta_j$, where $\nu_j \in \{0, 1\}$ are eigenvalues of $2n$ mutually commuting, non-Hermitian number operators $\hat{b}'_j \hat{b}_j$.

Let $|\mathrm{ness}\rangle$ be the element of $\mathcal{K}$ corresponding to the stationary solution ρ_{ness} (NESS) of Eq. (2), i.e., zero eigenvalue of $\hat{\mathcal{L}}$, $\nu_j \equiv 0$. The main result of Ref. [9] (Theorem 3) takes into account the fact that $|\mathrm{ness}\rangle$ is a right vacuum of $\hat{\mathcal{L}}$—the left vacuum being the trivial identity state $|\mathbb{1}\rangle$—and asserts that any quadratic physical observable can be explicitly computed in terms of eigenvectors $\underline{v}_p$, $\mathrm{tr}(w_j w_k \rho_{\mathrm{ness}}) = \delta_{j,k} + \langle \mathbb{1}|\hat{c}_j \hat{c}_k|\mathrm{ness}\rangle$,

$$\langle \mathbb{1}|\hat{c}_j\hat{c}_k|\mathrm{ness}\rangle = \frac{1}{2}\sum_{m=1}^{2n}(v_{2m,2j-1}v_{2m-1,2k-1} - v_{2m,2j}v_{2m-1,2k} - iv_{2m,2j}v_{2m-1,2k-1} - iv_{2m,2j-1}v_{2m-1,2k}). \quad (5)$$

Higher order observables can be computed using the Wick theorem. For example, noting $\sigma^z_m = -iw_{2m-1}w_{2m}$, the spin-spin correlator which we shall study later reads

$$\begin{aligned} C_{l,m} &= \mathrm{tr}(\sigma^z_l\sigma^z_m\rho_{\mathrm{ness}}) - \mathrm{tr}(\sigma^z_l\rho_{\mathrm{ness}})\mathrm{tr}(\sigma^z_m\rho_{\mathrm{ness}}) \\ &= \langle \mathbb{1}|\hat{c}_{2l-1}\hat{c}_{2m}|\mathrm{ness}\rangle\langle \mathbb{1}|\hat{c}_{2l}\hat{c}_{2m-1}|\mathrm{ness}\rangle - \langle \mathbb{1}|\hat{c}_{2l-1}\hat{c}_{2m-1}|\mathrm{ness}\rangle\langle \mathbb{1}|\hat{c}_{2l}\hat{c}_{2m}|\mathrm{ness}\rangle \quad \text{if} \quad l \neq m. \end{aligned} \quad (6)$$

As proven in Ref. [9], the NESS is unique iff the rapidity spectrum is nondegenerate, $\beta_j \neq 0$ for all j, and (almost) any initial state approaches NESS asymptotically exponentially with the rate $\Delta = 2\min_j \mathrm{Re}\beta_j$ if $\Delta > 0$.

Let us now proceed to detailed analytical and numerical investigation of the structure of the NESS in the XY chain. The bulk spectrum of rapidities for $n \to \infty$ is insensitive to the coupling to the baths and is given by $\beta = \pm i\epsilon(\phi)$, $\phi \in (-\pi, \pi]$, where $\epsilon(\phi) = [(\cos\phi - h)^2 + \gamma^2\sin^2\phi]^{1/2}$ is the quasiparticle dispersion relation in an infinite XY chain (see, e.g., [10]). For a finite chain (1) with the bath coupling on the edges (3), we find that the bulk (nearly continuous) rapidity spectrum gains a small never-vanishing real part $\mathrm{Re}\beta(\phi) = \mathcal{O}(n^{-1})$. At the spectral edges β^*, $\beta^*|_{n=\infty} = \pm i\epsilon(\phi^*)$, with ϕ^* defined by $d\epsilon(\phi^*)/d\phi = 0$, the gap is actually much smaller $\mathrm{Re}\beta^* = \mathcal{O}(n^{-3})$ (analytical result, generalizing [9]). Thus, the asymptotic relaxation time to NESS $1/\Delta = \mathcal{O}(n^3)$ diverges in the thermodynamic limit $n \to \infty$.

We note, however, that the structure of the quasiparticle spectrum $\epsilon(\phi)$ qualitatively changes as the magnetic field crosses a critical value

$$h_c(\gamma) = 1 - \gamma^2; \quad (7)$$

namely, for $h < h_c$ the minimal quasiparticle energy exists for a nontrivial value of quasimomentum $\phi^* = \arccos[h/h_c(\gamma)]$ yielding a new, nontrivial band edge β^*, whereas for $h > h_c$ the band edges can exist only at points $\phi^* = 0, \pi$ (see Fig. 1). Consequently, complex rapidities of an open XY chain shape up a third condensation point near the imaginary axis for $h < h_c$ which is composed of NMMs (eigenvectors of $\mathbf{A}$) with quasimomenta near $\phi^* \neq 0, \pi$ and has a dramatic effect on the structure of the NESS as we demonstrate below.

Indeed, as $h < h_c$, we find the emergence of long-range magnetic correlations (LRMCs) characterized by nondecaying structures in the correlation matrix $C_{l,m}$ (6). The typical size ℓ of the correlation patches is of the order $\ell \sim 1/\phi^*$ (Fig. 2). For $h \approx h_c$ one finds critical scaling $\phi^* \approx [2(h_c - h)/h_c]^{1/2}$, which agrees with the data.

In the critical case $h = h_c$ [see Fig. 3(a)], one finds power-law decay of the correlation matrix $C_{l,m} \propto |l - m|^{-4}$ if neglecting finite size or boundary effects. If we scale the distance, we find numerically a finite size scaling $n^\nu C_{l,m} = f(|l - m|/n)$, where $\nu = 4.09$ and $f(x)$ is some function describing data for all large n [inset in Fig. 3(a)]. Critical point $h = h_c$ is also characterized by faster closing of the spectral gap Δ of Liouvillean; namely, there we find $\mathrm{Re}\beta^* = \mathcal{O}(n^{-5})$, meaning n^2 times longer relaxation times of generic solutions $\rho(t)$ of (2).

For $h > h_c$, we have $\phi^* = 0$ and no LRMC in NESS. Then one finds an exponential decay of the correlation matrix $C_{l,m} \propto \exp(-|l - m|/\xi)$ with the localization length which can be estimated theoretically from a scattering problem defined by the matrix (4): $\xi^{-1} = 4\cosh^{-1}(h/h_c) \approx 4[2(h - h_c)/h_c]^{1/2}$, where the factor 4 reflects the fact that $C_{l,m}$ is a 4-point function in NMM amplitudes $\underline{v}_p$ [see Fig. 3(b)].

The above results are summarized in a nonequilibrium phase diagram of the XY chain (Fig. 4) showing the residual correlator $C_{\mathrm{res}} = \sum_{l,m}^{|l-m|>n/2} C_{l,m}/\sum_{l,m}^{|l-m|>n/2} 1$ (which is found to be always negative) in the γ-h plane, with the critical curve $h_c(\gamma)$ separating the two phases. Note that

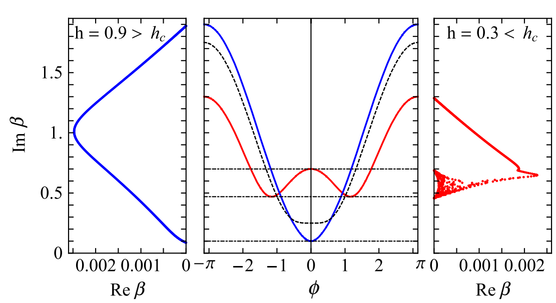

FIG. 1 (color online). Rapidity spectrum $\{\beta_j\}$ around the imaginary axis for $n = 640$, $\Gamma^L_1 = 0.5$, $\Gamma^L_2 = 0.3$, $\Gamma^R_1 = 0.5$, $\Gamma^R_2 = 0.1$, $\gamma = 0.5$, and $h = 0.3 < h_c$ (left, blue curve) and $h = 0.9 > h_c$ (right, red curve), compared to the free XY dispersion $\epsilon(\phi)$ (center), dashed curve indicating the critical case $h = h_c$.

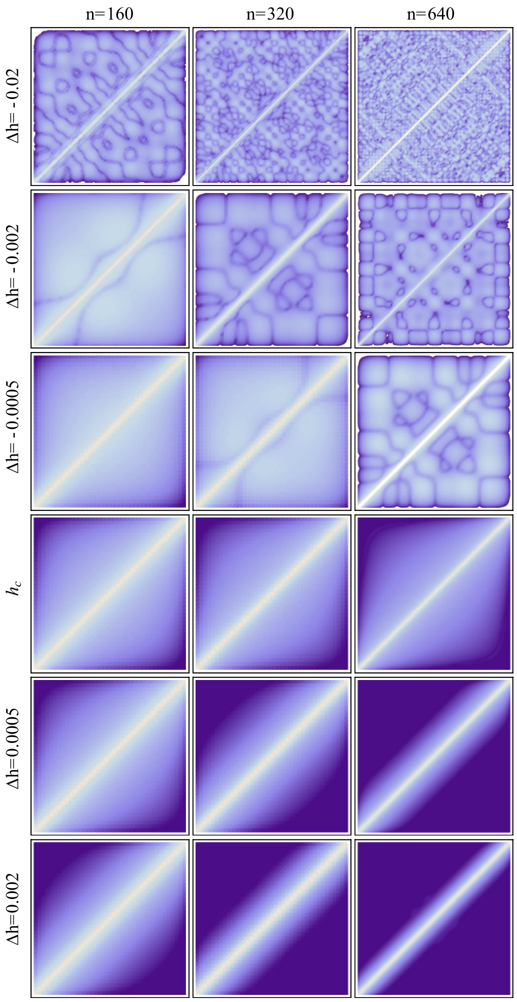

FIG. 2 (color online). Spin-spin correlation matrices (6) for three different sizes n (columns) and different values of $\Delta h = h - h_c$ (rows) surrounding the critical value (7). γ and Γ^{λ}_{μ} are the same as in Fig. 1. The color scale is proportional to $\log|C_{l,m}|$ and ranges from $\log 10^{-18}$ (dark blue) to log1 (white).

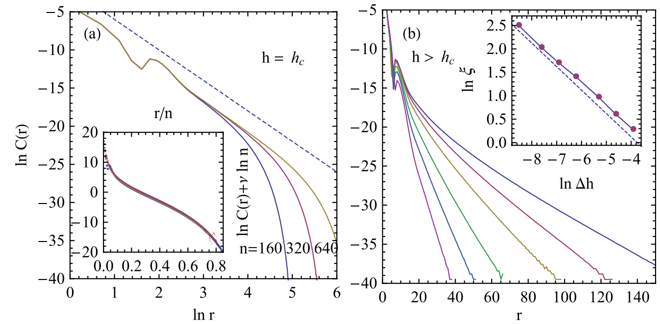

FIG. 3 (color online). Spin-spin correlator $C(r)$ computed as an average of $C_{l,m}$ with fixed $r = |l - m|$ and $|l + m - n| \leq 0.08n$. In (a) we plot $C(r)$ in the critical case $h = h_c = 0.75$ (γ and Γ^{λ}_{μ} are the same as in Fig. 1) for several sizes $n = 160$, 320, and 640 (indicated), while the dashed line indicates asymptotic r^{-4} decay. The inset shows the scaled correlator $n^{\nu}C(r)$ versus r/n with $\nu = 4.09$ for the same data. In (b) we plot $C(r)$ for changing $h = 0.7505, 0.751, 0.752, 0.755, 0.76, 0.77 > h_c$ (right-to-left colored curves). The inset shows numerically determined localization length ξ versus $\Delta h = h - h_c$ (points) as compared to theoretical estimate [see text] (dashed line).

the other boundary lines $\gamma = 0$ (XX chain) and $h = 0$ (XY with zero field) are not in the LRMC phase.

In analogy to equilibrium QPTs [11,12], we wish to characterize the nonequilibrium transition in terms of quantum information theoretic concept, namely, with the difficulty of classical simulation of ρ_{ness} which is described in terms of the OSEE [13] (or block entropy in $\mathcal{K}$), i.e., von Neumann entropy $S(n) = -\mathrm{tr}_{[1,n/2]}\hat{R}\log_2\hat{R}$ of the reduced density matrix of a half-chain $\hat{R} = \mathrm{tr}_{[n/2+1,n]}|\mathrm{ness}\rangle\langle\mathrm{ness}|$. $\mathrm{tr}_{[j,k]}$ is a partial trace over the sublattice $[j, k]$. Straightforward calculation, combining Refs. [9,12], results in $S(n) = -\sum_{j=1}^{n}[(\frac{1}{2} + \eta_j) \times \log_2(\frac{1}{2} + \eta_j) + (\frac{1}{2} - \eta_j)\log_2(\frac{1}{2} - \eta_j)]$, where η_j are n positive eigenvalues of an upper-left $2n \times 2n$ [14] block of $4n \times 4n$ Hermitian matrix $\mathbf{D}_{pq} = \langle\mathrm{ness}|\hat{a}_p\hat{a}_q|\mathrm{ness}\rangle/\langle\mathrm{ness}|\mathrm{ness}\rangle$. $\mathbf{D}$ can be computed by expressing $\hat{a}_p$ in terms of NMM maps $\hat{b}_j$ and $\hat{b}^{\dagger}_j$ (not $\hat{b}'_j$), $\underline{\hat{a}} = \mathbf{Q}^*\underline{\hat{b}} + \mathbf{Q}\underline{\hat{b}}^{\dagger}$, as $\mathbf{D} = \mathbf{Q}^*\mathbf{T}\mathbf{Q}^T$, where $T_{j,k} = \sum_{p=1}^{4n} v_{2j-1,p}v^*_{2k-1,p}$ is a $2n \times 2n$ matrix and $\mathbf{Q} = \mathbf{V}_o\mathbf{K}_{12}$, where $\mathbf{K}_{12}$ designates the upper-right $2n \times 2n$ quarter of $4n \times 4n$ matrix $\mathbf{K} = -(\mathbf{V}_o| - \mathbf{V}^*_o)^{-1}(\mathbf{V}_e| - \mathbf{V}^*_e)$ and $(\mathbf{V}_e)_{p,k} = v_{2k,p}$, $(\mathbf{V}_o)_{p,k} = v_{2k-1,p}$ are $4n \times 2n$ matrices. $(\mathbf{X}|\mathbf{Y})$ denotes the vertical concatenation of two $4n \times 2n$ matrices into a single $4n \times 4n$ matrix.

The resulting behavior of $S(n)$ in the NESS of the XY chain is striking (see Fig. 5): LRMC phase $h < h_c$ is characterized with a linear growth $S(n) = sn + \mathrm{const}$, with some constant $s > 0$. This has to be contrasted with a $\log n$ growth found for equilibrium critical models [12]. As h approaches h_c, the slope s approaches 0 as $s \propto (h_c - h)^{\tau}$, with numerically determined critical exponent $\tau \approx 0.80$, and the fluctuations of $S(n)$ around an average linear growth increase. These fluctuations can be explained by the sensitive dependence of NESS on boundary conditions (bath couplings or size changes) due to long-range correlations, evident also in the structures of the correlation matrices (Fig. 2). Note also an interesting "quantization of bipartite entanglement" which is observed for very small $h_c - h$ where $S(n)$ can take only approximately a discrete set of values $S(n) \approx S_0 + k$, $k \in \mathbb{Z}^+$ and which can be explained by the quasiparticle picture of the NMM. At and above the critical field $h \geq h_c$, we find saturation $S(n) = \mathcal{O}(1)$ and vanishing fluctuations of $S(n)$, since there the NESS becomes insensitive to boundary conditions due to fast decay of magnetic correlations. Only there can the NESS be efficiently simulated, e.g., in terms of matrix product states [15], by numerical methods such as the density matrix renormalization group (DMRG) [16].

All of the numerical results presented above have been obtained for fixed nonequilibrium bath couplings $\Gamma^L_1 = 0.5$, $\Gamma^L_2 = 0.3$, $\Gamma^R_1 = 0.5$, and $\Gamma^R_2 = 0.1$. However, the results did not change qualitatively, in particular, the phase boundary, when we (i) varied the bath couplings Γ^{λ}_{μ} [8],

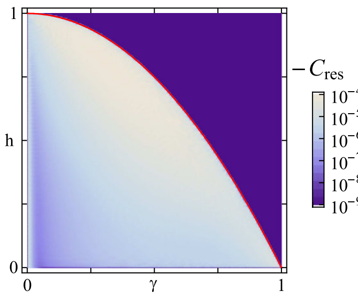

FIG. 4 (color online). Phase diagram γ-h showing the residual correlator $-C_{\rm res}$ (log scale indicated) for size $n = 160$ (Γ_μ^λ as in Fig. 1). The red curve is the critical line (7). Note that $C_{\rm res}$ is practically insensitive to increasing n in the LRMC phase (bright).

(ii) coupled several spins around each end to Lindbladian baths, or (iii) even set the bath couplings equal $\Gamma_\mu^L = \Gamma_\mu^R$. The latter case (iii) does not represent an equilibrium situation; i.e., $\rho_{\rm ness}$ is not a thermal state $\rho_T = Z^{-1} \times \exp(-H/T)$ as the XY chain is not ergodic [10]. For example, no discontinuity at $h = h_c$ appears in the properties of ρ_T for any T, and correlator $C(r)$ decays with T-dependent rates [10], whereas in the non-LRMC phase of the NESS decay length ξ is asymptotically insensitive to bath parameters. Furthermore, thermal states in one dimension have bounded OSEE in n [17] and related quantities [18]; hence, the simulation complexity of NESS is qualitatively different.

In spite of the demonstrated discontinuity in the spin-spin correlation function, the local observables such as energy or spin density in the NESS are numerically found to be smooth functions of h at h_c, so the nonequilibrium transition appears to be of high or infinite order (similar to the Kosterlitz-Thouless transition). The LRMC phase could perhaps be difficult to detect experimentally as the residual

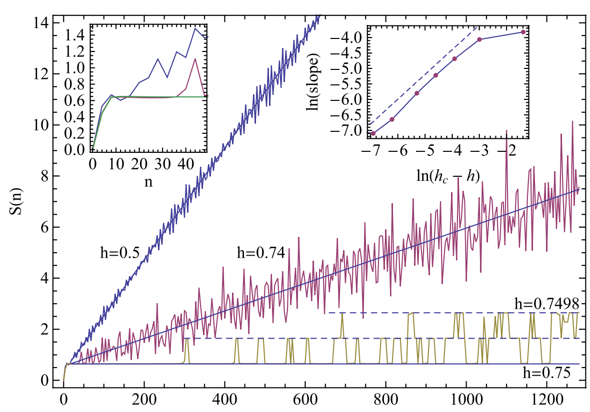

FIG. 5 (color online). OSEE $S(n)$ (symmetric chain bipartition) for γ and Γ_μ^λ of Fig. 1 and different $h \le h_c = 0.75$ (indicated). The best fitting linear growths are indicated with straight lines. Dashed horizontal lines indicate $S_0 + 1$ and $S_0 + 2$, S_0 being the saturation value for $h = h_c$. The left inset just magnifies the scale, while the right inset shows the slope of $S(n)$ growth vs $h_c - h$ (log-log), and $|h_c - h|^{0.8}$ (dashed line).

correlation $C_{\rm res}$ is not larger than a few times 10^{-4} (Fig. 4) even in the optimal case (with respect to varying Γ_μ^λ).

In conclusion, we report on the QPT in the NESS of an open quantum XY spin chain, whose theoretical and numerical description is formally analogous to equilibrium QPTs in spin chains at zero temperature inasmuch as the NESS can formally be treated as a "ground state" of the quantum Liouvillean. We show that the phase transition is of mean-field type as the quasiparticle picture gives a satisfactory theoretical description, in particular, the phase boundary between long-range and exponentially decaying magnetic correlations. We demonstrate that the two phases, respectively, correspond to linearly growing and saturating entanglement entropy of the NESS in operator space as a function of the chain length. This behavior is drastically different than in equilibrium XY chains.

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